Uncertainty quantification of UNEDF EDF models and lessons learned for novel EDF development

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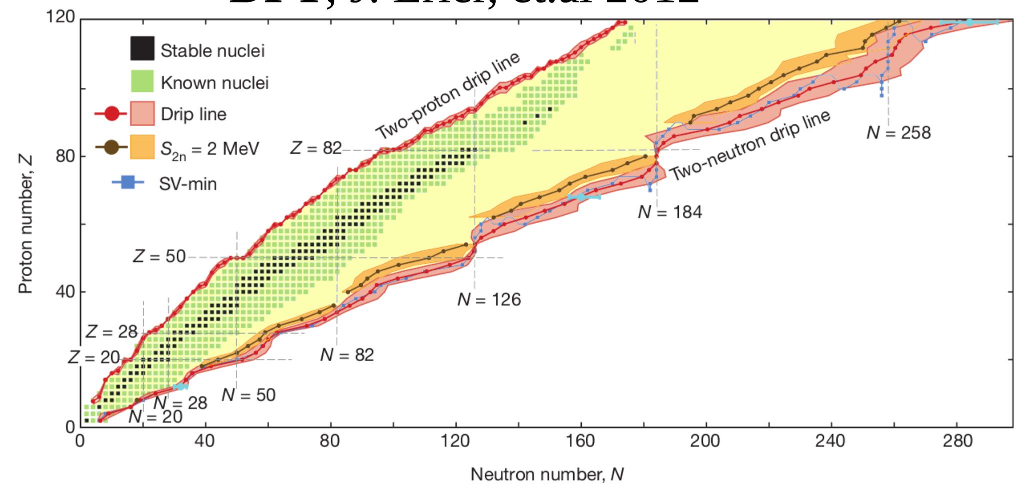
Nuclear density functional theory

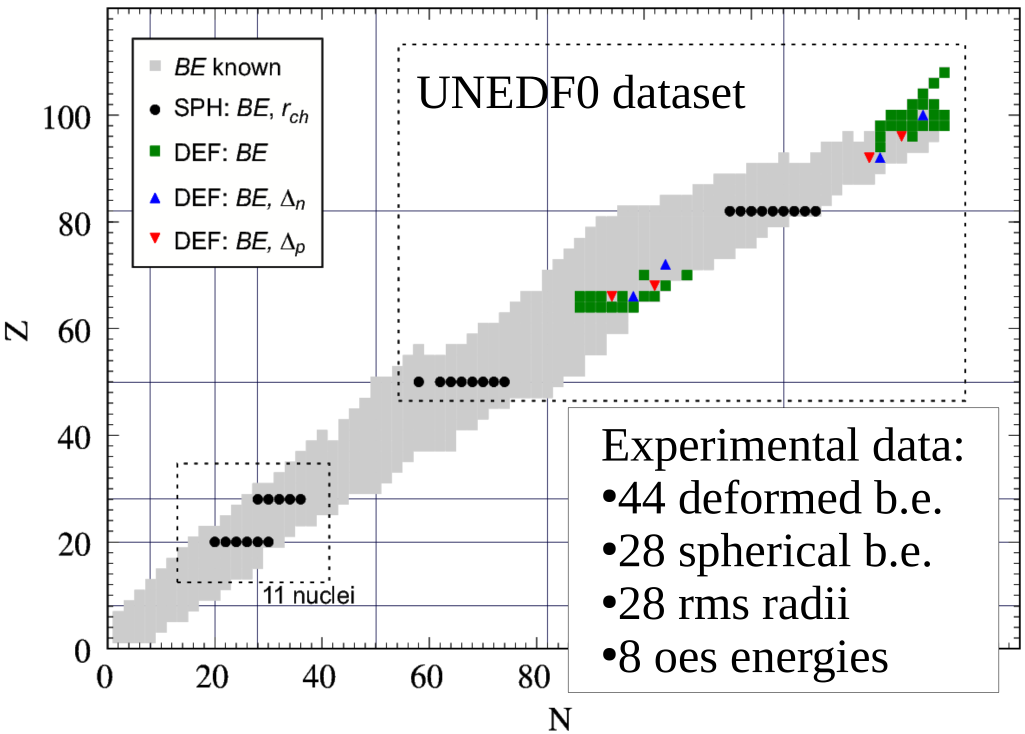
- The nuclear DFT is the only microscopic theory which can be applied throughout the entire nuclear chart
- Important ingredient of DFT: The energy density functional (EDF)
- EDF incorporates complicated many-body correlations into a function composed of nuclear densities and currents
- Hohenberg-Kohn theorem: There exists universal EDF applicable for all systems
- In practice EDF is usually constructed from some ansatz containing adjustable parameters
- EDF parameters can not be obtained from any theory withing required accuracy: They are adjusted to empirical input

DFT, J. Erler, et.al 2012



- Goal with nuclear EDF development: An universal EDF, applicable throughout the nuclear chart, reproducing various kind of experimental data

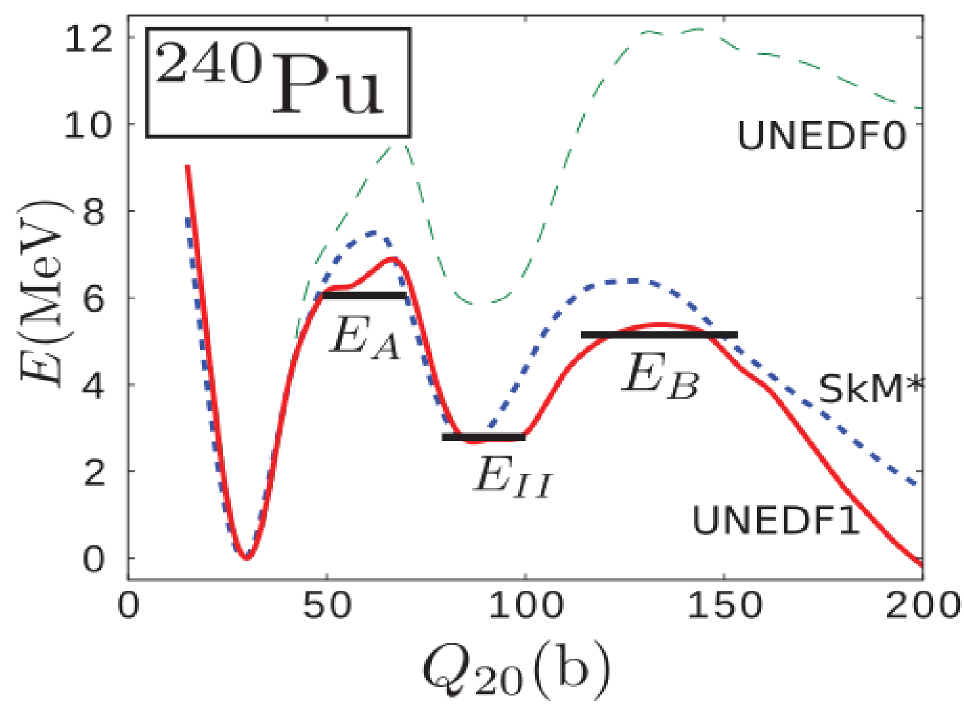
Energy density optimization: UNEDF0 and UNEDF1



UNEDF0: M. K., T. Lesinski, J. Moré, W. Nazarewicz, J. Sarich, N. Schunck, M. V. Stoitsov, S. Wild, PRC 82, 024313 (2010)

UNEDF1: M. K., J. McDonnell, W. Nazarewicz, P.-G. Reinhard, J. Sarich, N. Schunck, M. V. Stoitsov, S. Wild, PRC 85, 024304 (2012)

- UNEDF1 was the first parameterization which was systematically optimized at the deformed HFB level for fission studies
- UNEDF1 included data on 4 fission isomers states (^{226}U, ^{238}U, ^{240}Pu, ^{242}Cm), in addition to UNEDF0 data set



- χ^2-optimization of Skyrme-like ED with respect of 12 parameters at the deformed HFB level

$$\rho_c, E^{NM}/A, K^{NM}, a_{sym}^{NM}, L_{sym}^{NM}, M_s^{-1}$$
$$C_0^{\rho\Delta\rho}, C_1^{\rho\Delta\rho}, V_0^n, V_0^p, C_0^{\rho\nabla J}, C_1^{\rho\nabla J}$$

- UNEDF0 input data consisted of masses of deformed and spherical nuclei, charge radii, and pairing gaps
- Only time-even part of the EDF was adjusted for all UNEDF's

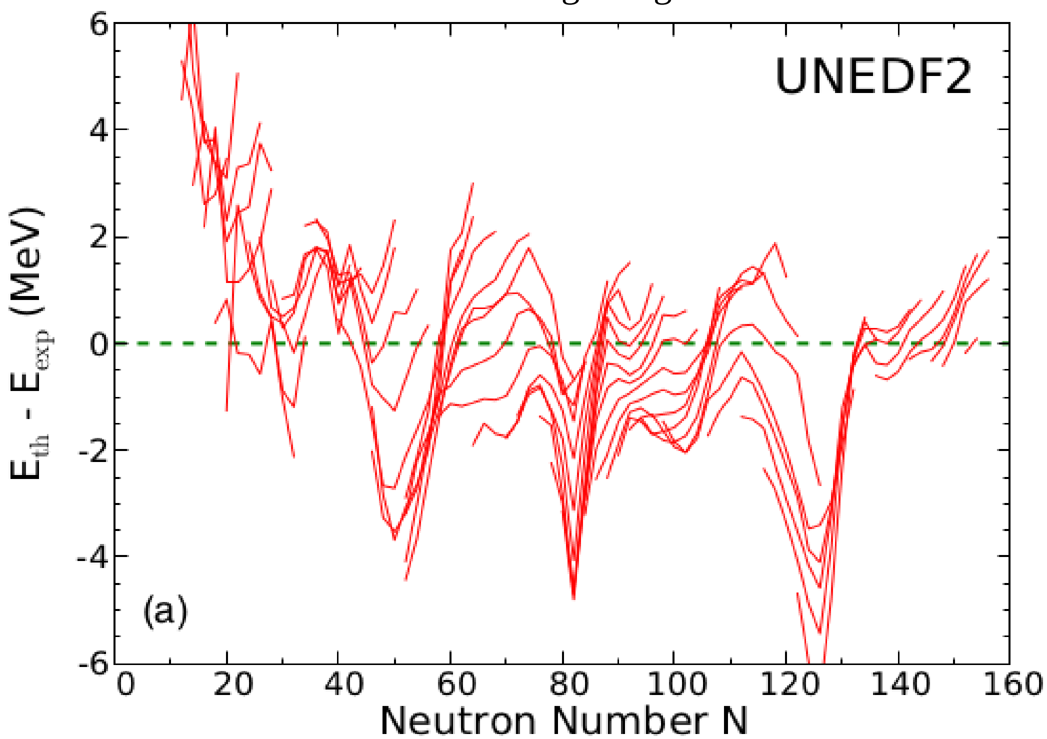
Energy density optimization: UNEDF2

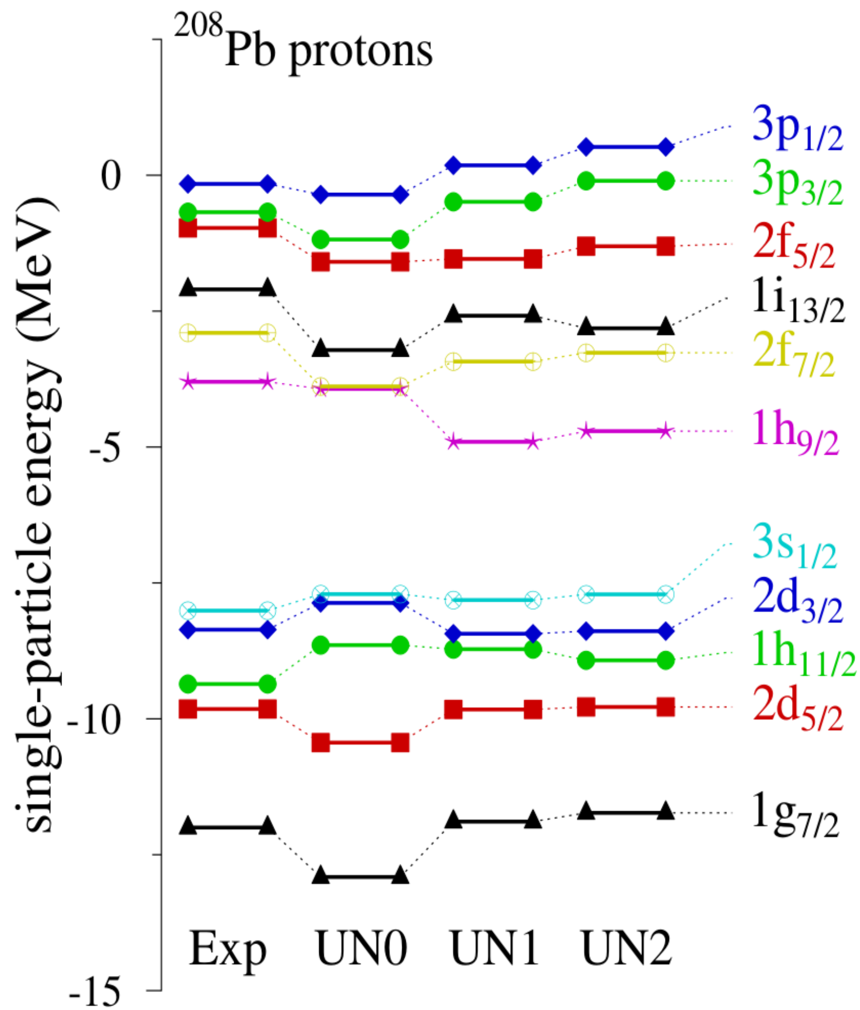
- Optimization of Skyrme-like ED with respect of 14 parameters at deformed HFB level: Tensor terms now included

$$\rho_c, E^{NM}/A, K^{NM}, a^{NM}_{sym}, L^{NM}_{sym}, M_s^{-1}$$
$$C_0^{\rho\Delta\rho}, C_1^{\rho\Delta\rho}, V_0^n, V_0^p, C_0^{\rho\nabla J}, C_1^{\rho\nabla J}, \boxed{C_0^J, C_1^J}$$

- Focus on shell structure: Single particle energies included in the optimization. These are handled with blocked HFB calculations

UNEDF2 binding energies





UNEDF2: M.K., J. McDonnell, W. Nazarewicz, E. Olsen, P.-G. Reinhard, J. Sarich, N. Schunck, S.M. Wild, D. Davesne, J. Erler, A. Pastore, Phys. Rev. C 89 054314 (2014)

Performance of UNEDF EDFs

RMS deviations of various observables (in units of MeV or fm)

Observable	UNEDF0	UNEDF1	UNEDF2	No.
E	1.428	1.912	1.950	555
E $(A < 80)$	2.092	2.566	2.475	113
E $(A \geqslant 80)$	1.200	1.705	1.792	442
S_{2n}	0.758	0.752	0.843	500
S_{2n} $(A < 80)$	1.447	1.161	1.243	99
S_{2n} $(A \geqslant 80)$	0.446	0.609	0.711	401
S_{2p}	0.862	0.791	0.778	477
S_{2p} $(A < 80)$	1.496	1.264	1.309	96
S_{2p} $(A \geqslant 80)$	0.605	0.618	0.572	381
$\tilde{\Delta}_n^{(3)}$	0.355	0.358	0.285	442
$\tilde{\Delta}_n^{(3)}$ $(A < 80)$	0.401	0.388	0.327	89
$\tilde{\Delta}_n^{(3)}$ $(A \geqslant 80)$	0.342	0.350	0.273	353
$\tilde{\Delta}_p^{(3)}$	0.258	0.261	0.276	395
$\tilde{\Delta}_p^{(3)}$ $(A < 80)$	0.346	0.304	0.472	83
$\tilde{\Delta}_p^{(3)}$ $(A \geqslant 80)$	0.229	0.248	0.194	312
R_p	0.017	0.017	0.018	49
R_p $(A < 80)$	0.022	0.019	0.020	16
R_p $(A \geqslant 80)$	0.013	0.015	0.017	33

RMS deviations of single particle energies (in MeV)

Nuclei	UNEDF0	UNEDF1	UNEDF2
All	1.42	1.38	1.38
Light	1.80	1.72	1.74
Heavy	0.94	0.97	0.95

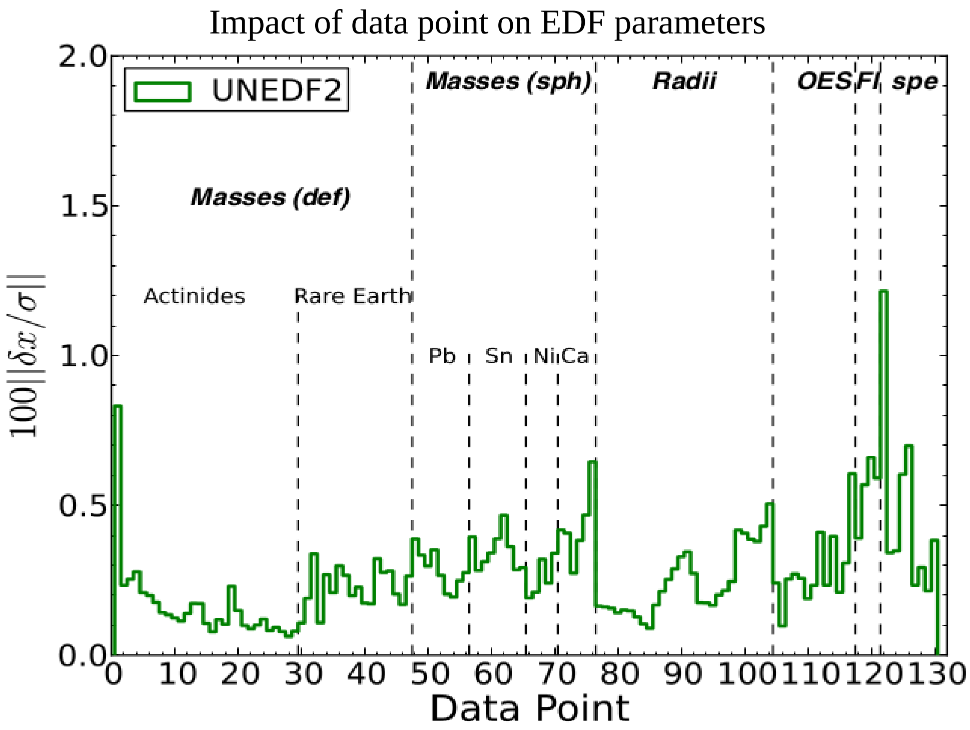
(best attainable RMS deviation for Skyrme s.p. energies is around 1.1-1.2 MeV)

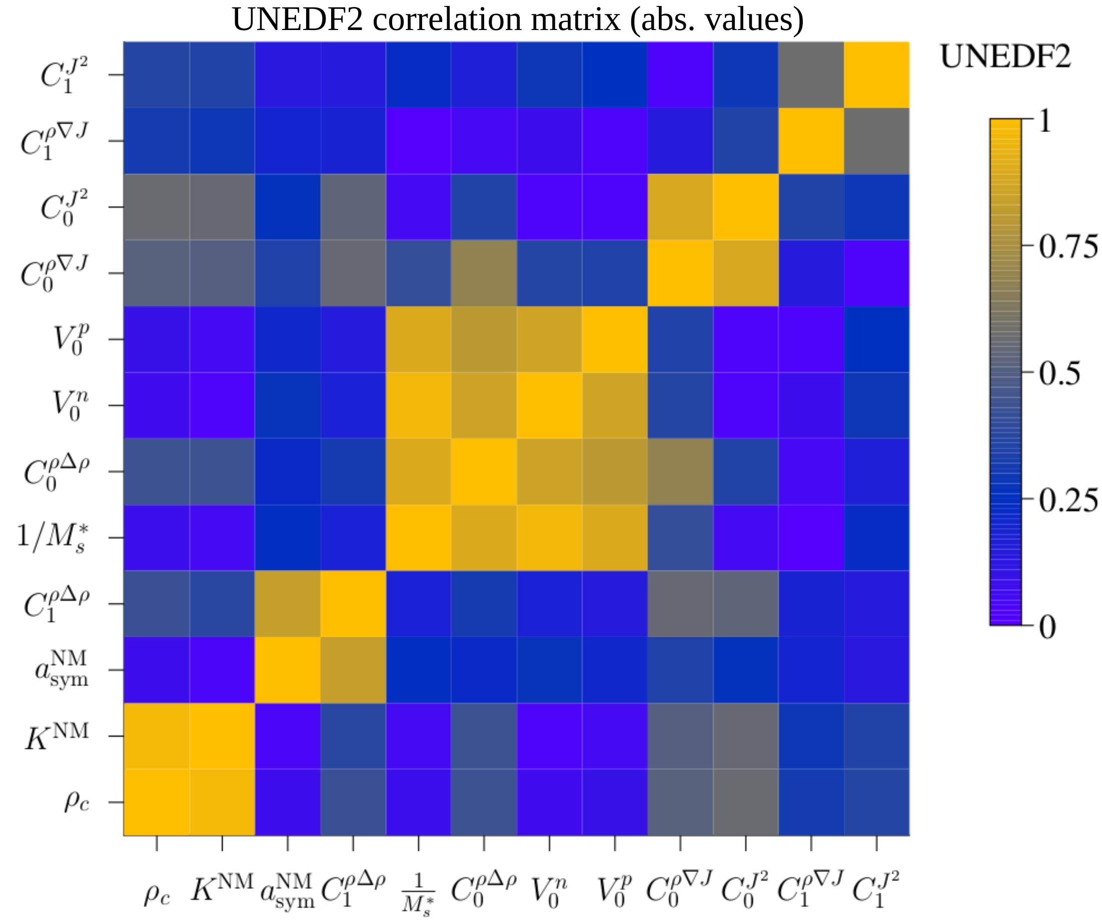
RMS deviations inner (A) and outer (B) and fission barrier height, and fission isomer (I) energy (in MeV)

	UNEDF2	UNEDF1	FRLDM	SkM*	D1S
E_{A}	1.470	1.030	1.520	1.610	0.709
E_{II}	0.515	0.357	0.675	0.351	0.339
E_{B}	1.390	0.690	1.130	1.390	1.140

- Generally, UNEDF2 gives no or only marginal improvement over to UNEDF1 ⇒ Novel EDF developments required to improve precision

Sensitivity analysis





- With UNEDF0,1 and 2, a complete sensitivity analysis was done for the obtained χ^2 minimum, providing standard deviations and correlations of the model parameters
- Sensitivity analysis can also tell what is the impact of given data point to the position of minimum
- During UNEDF EDF optimization, parameters had certain boundary values
- If model parameter must stay within some bounds, and these bounds do not include χ^2 minimum, sensitivity analysis can not be done for this parameter
- May have impact when computing error propagation for various observables

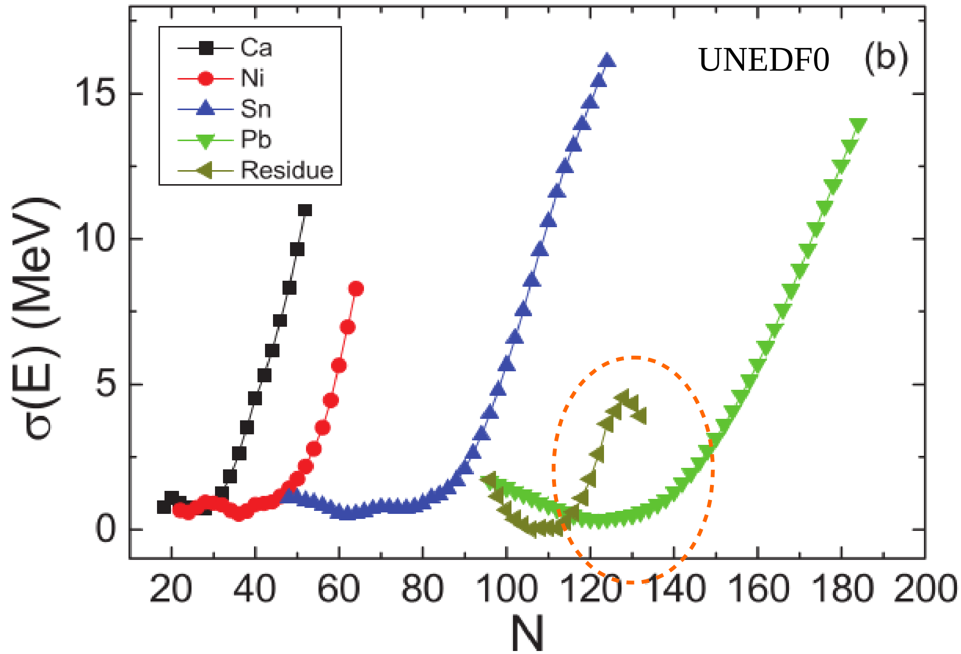
Uncertainty quantification

- Uncertainty quantification allows to assess predictive power of the model, i.e. how much can we trust predicted quantities
- Standard deviation of some observable *y* can be calculated by using covariance matrix of the model parameters

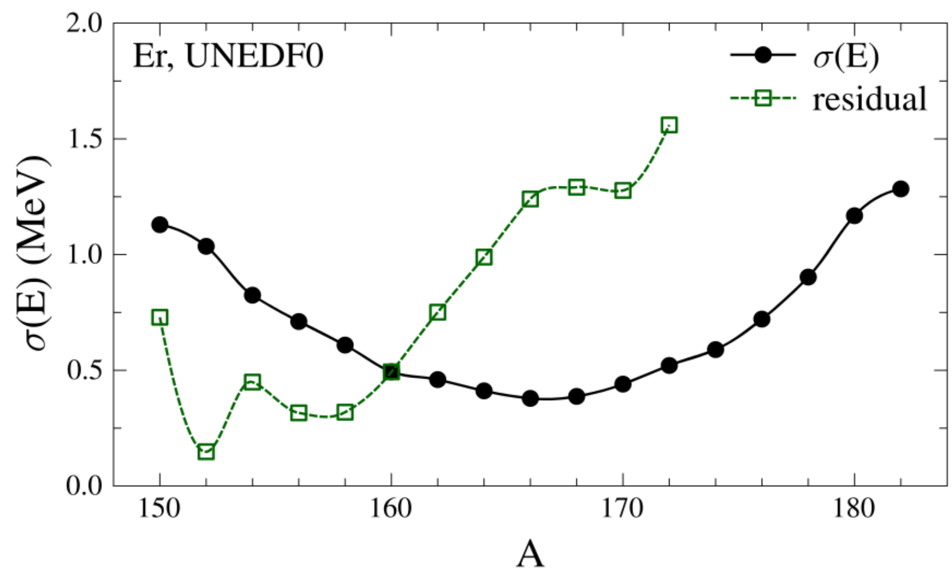
$$\sigma_y^2 = \sum_{i,j} \mathrm{Cov}(x_i, x_j) \left[\frac{\partial y}{\partial x_i} \frac{\partial y}{\partial x_j} \right]$$

- For some of the binding energies, statistical error is significantly smaller compared to residue from experimental data
  - Indication of deficiency of the model
  - “Model is blind to its own shortcomings”
- General trend is that propagated error increases sharply towards neutron rich nuclei: Badly constrained isovector part of the EDF
- Another uncertainty component is the systematic error. Much harder to quantify

Y. Gao, J. Dobaczewski, M. K., J. Toivanen, D. Tarpanov, PRC87, 034324 (2013)

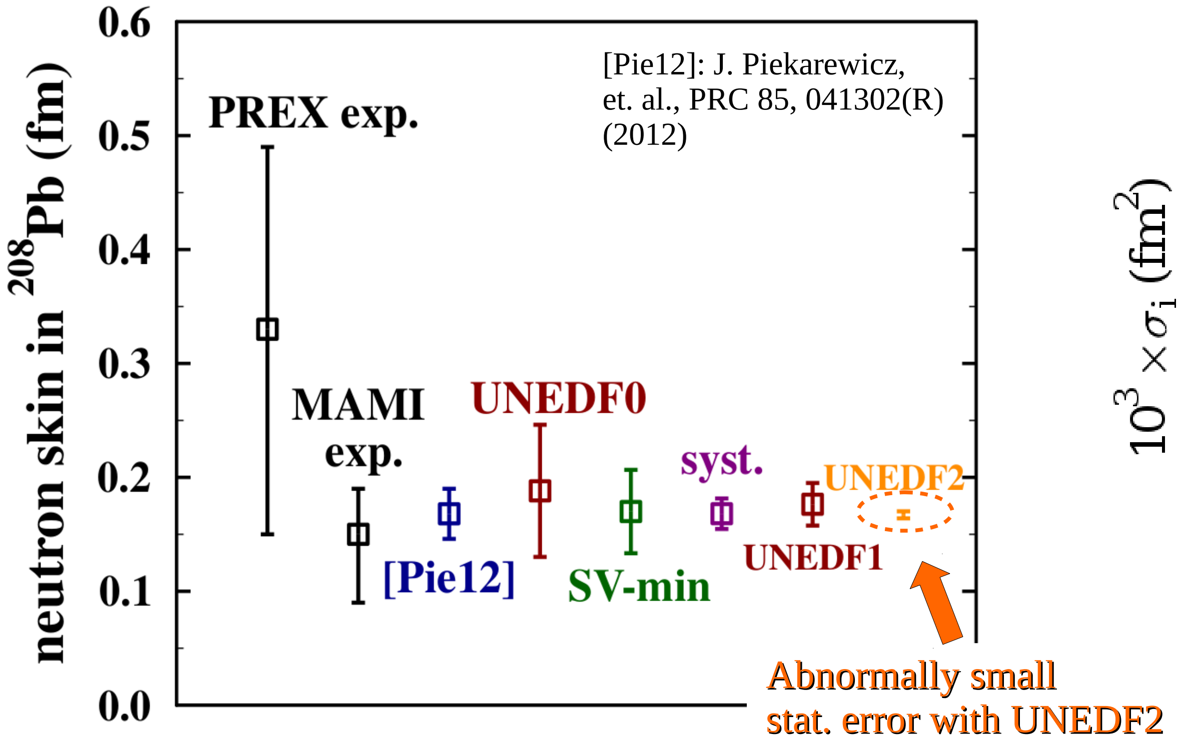


M. K., J. Phys. G 42, 034021 (2015)

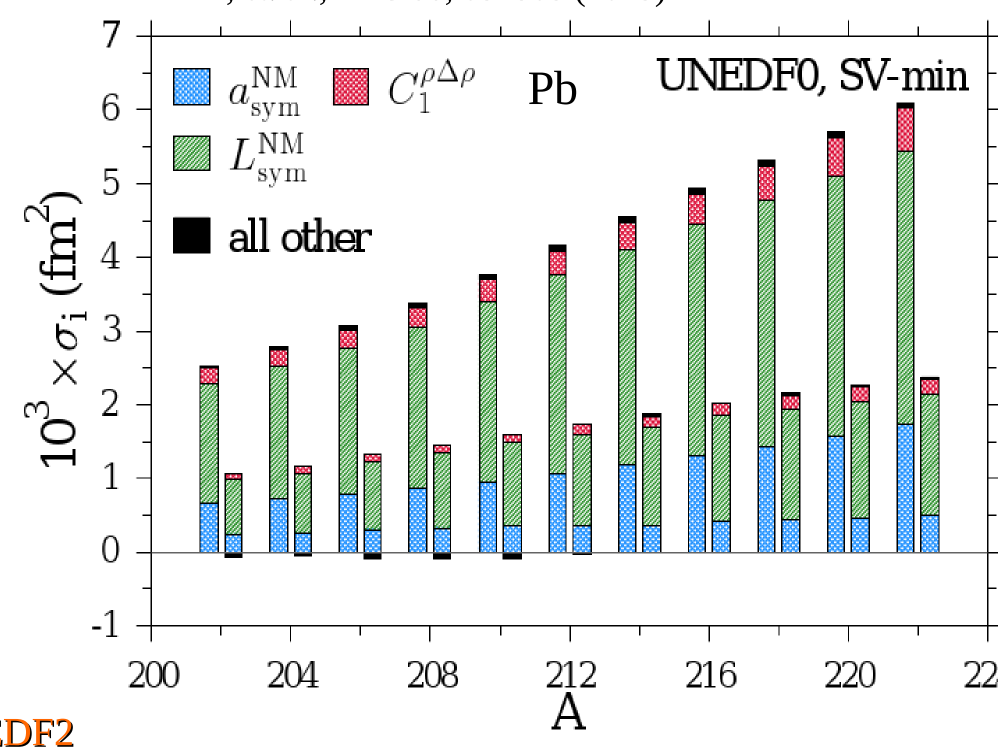


Neutron skin thickness

- Neutron skin thickness in ^{208}Pb was recently measured in P-REX and MAMI experiments. This gives valuable information about the neutron matter equations of the state
- P-REX experimental error bar larger than model uncertainties, MAMI error bar similar in magnitude compared to statistical model error
- Statistical uncertainty comes mostly from the uncertainty related to the density dependence of the symmetry energy. This reflects to uncertainty of the neutron matter density.
- With UNEDF2 L_{sym} was excluded from sensitivity analysis, since it hit the boundary value during optimization process. $\Rightarrow$ Abnormally small statistical error for neutron skin thickness.

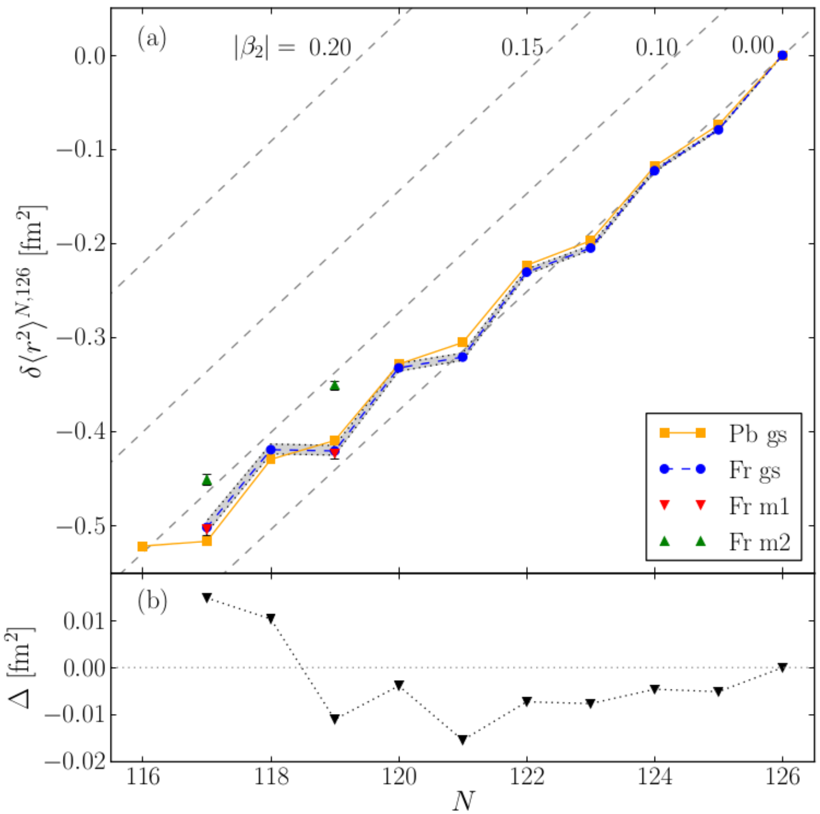


MK, et. al., PRC 88, 031305 (2013)



Charge radii of light Fr isotopes

A. Voss, et.al, Phys. Rev. C **91**, 044307 (2015)



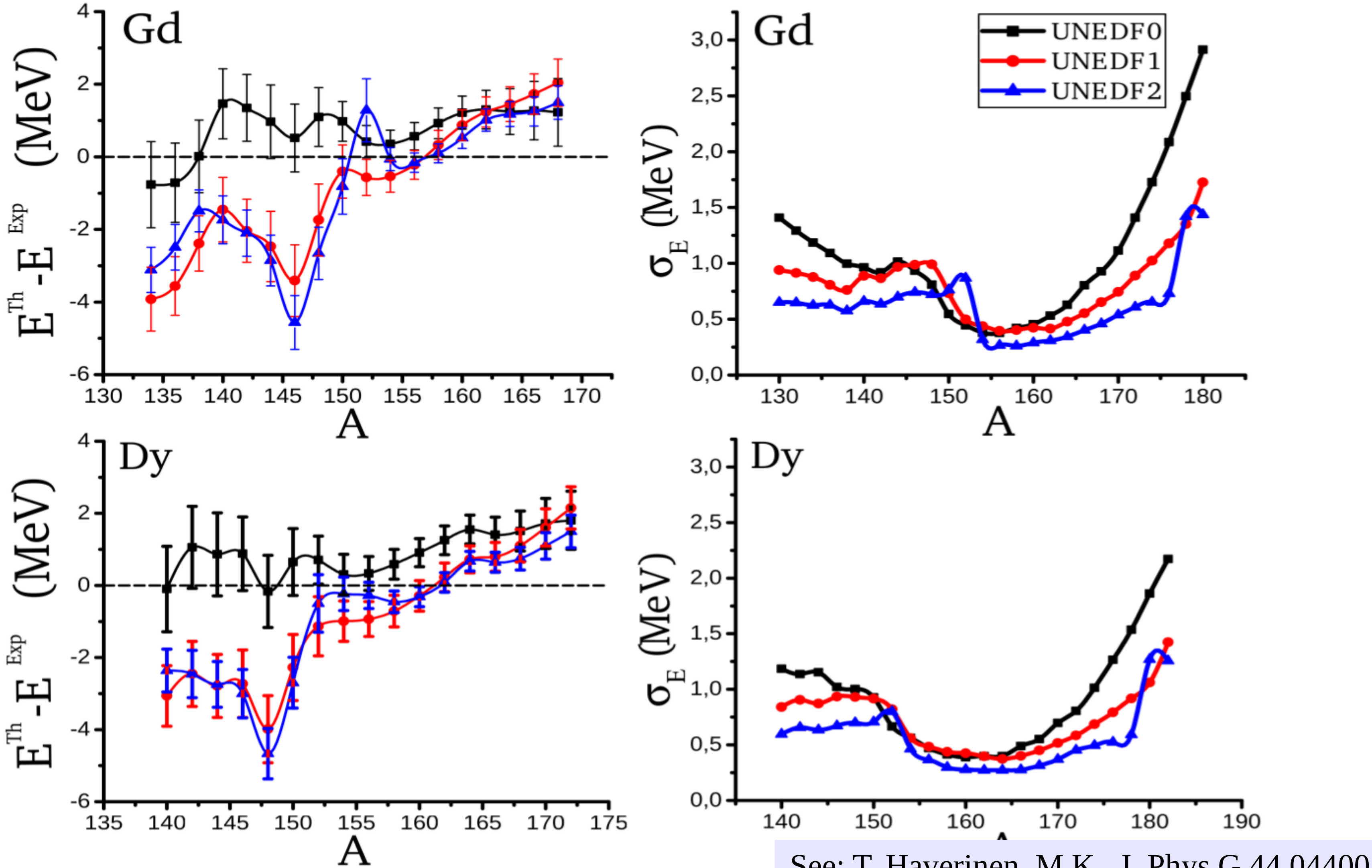
Charge radii and binding energies of Fr isotopes

A	$\langle r_{ch}\rangle$ (fm)		B (GeV)	
	EDF	Expt.	EDF	Expt.
213	5.576(6)	5.577	−1.65714(49)	−1.65468(1)
212	5.573(6)	5.570	−1.64825(52)	−1.64657(1)
211	5.567(6)	5.566	−1.64046(57)	−1.63912(1)
210	5.563(5)	5.559	−1.63109(63)	−1.63024(1)
209	5.561(5)	5.556	−1.62270(73)	−1.62261(1)
208	5.560(5)	5.548	−1.61336(76)	−1.61344(1)
207	5.557(5)	5.547	−1.60483(79)	−1.60554(2)
206	5.556(5)	5.539	−1.59535(81)	−1.59587(3)
205	5.554(5)	5.539	−1.58686(87)	−1.58787(1)
204	5.551(5)	5.532	−1.57721(91)	−1.57788(2)

- Charge radii of light Fr isotopes were recently measured at TRIUMF. This allowed to test predictive power of the UNEDF0 model
- Comparison to UNEDF0 prediction shows that even though binding energies can be reproduced well, charge radii of the lightest Fr isotopes could not be reproduced so well

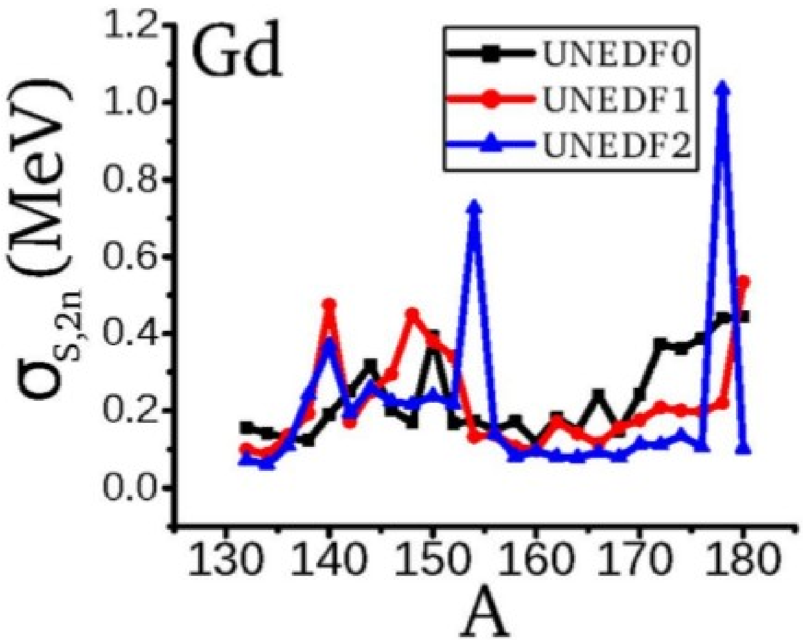
Uncertainty propagation in deformed rare earth nuclei, binding energy

- Propagated statistical uncertainties for rare earth binding energies follow similar patter to those in semi magic nuclei: Nuclei far from stability have larger theoretical uncertainties
- The latter the UNEDF model, the smaller are the uncertainties. However, best correspondence with experimental values is with UNEDF0

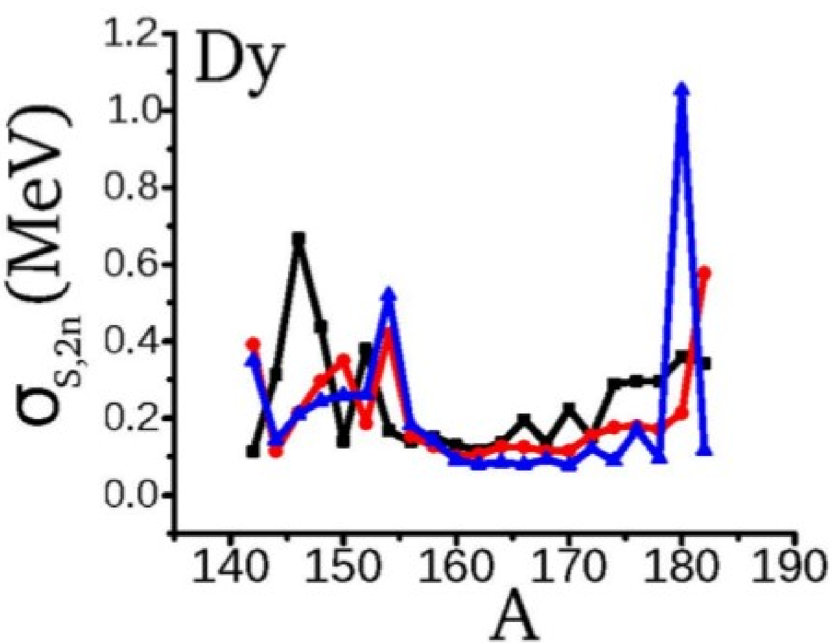


See: T. Haverinen, M.K., J. Phys G 44 044008 (2017)

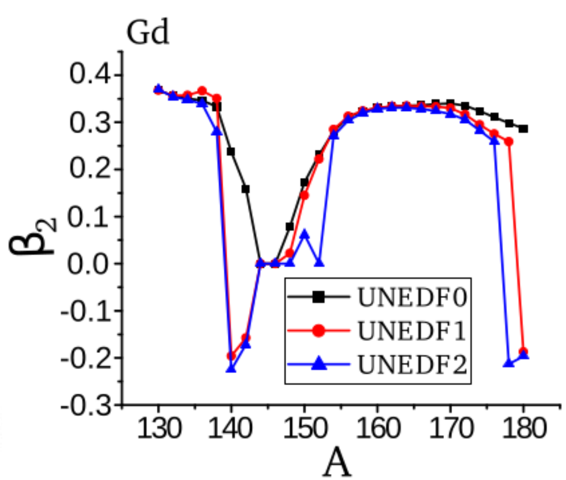
Uncertainty propagation in deformed rare earth nuclei, S_{2n} value



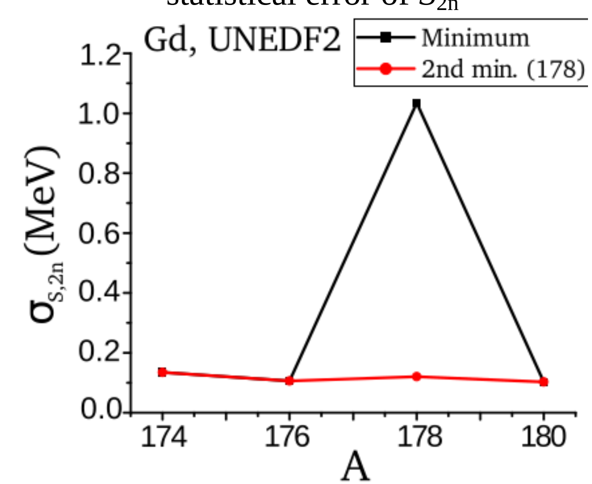
- Generally, with two-neutron separation energies, the statistical uncertainty is smaller compared to binding energies. Some of the uncertainties with isovector part are canceled out
- Statistical uncertainty has some sudden large values with some particular isotopes
- These are connected to a sudden change of deformation
- For example, deformation has a sudden change at A=178 with UNEDF2
- By using the secondary minimum of this nucleus, the deformation change is small and propagated error is similar to neighboring nuclei



Intrinsic deformation

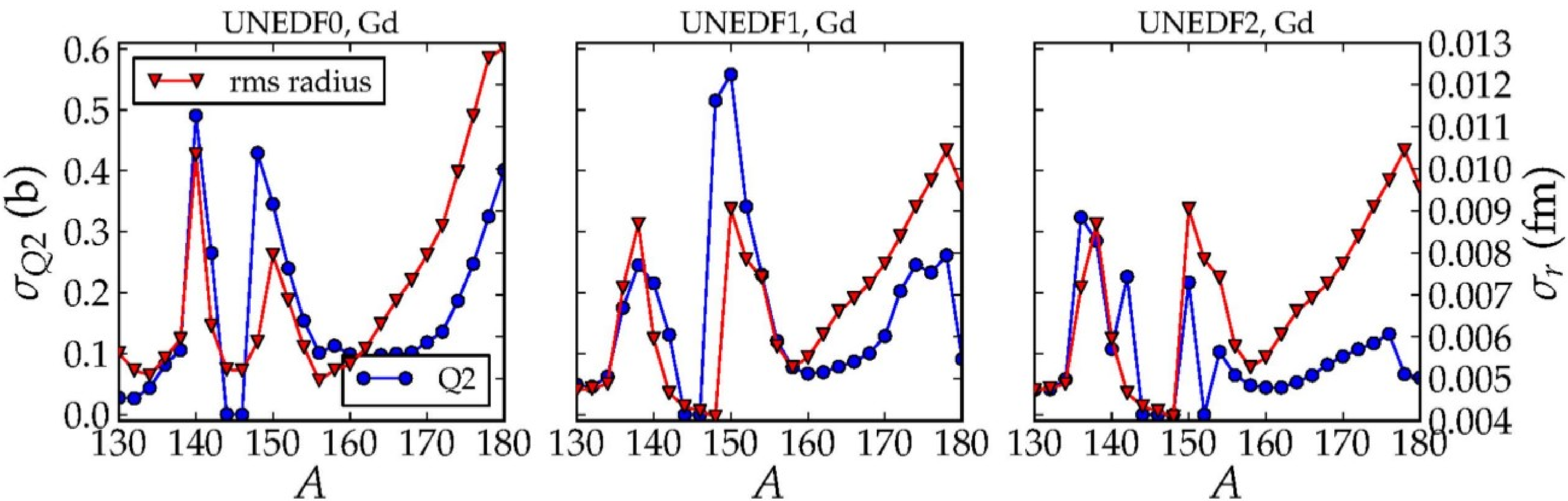


statistical error of S_{2n}

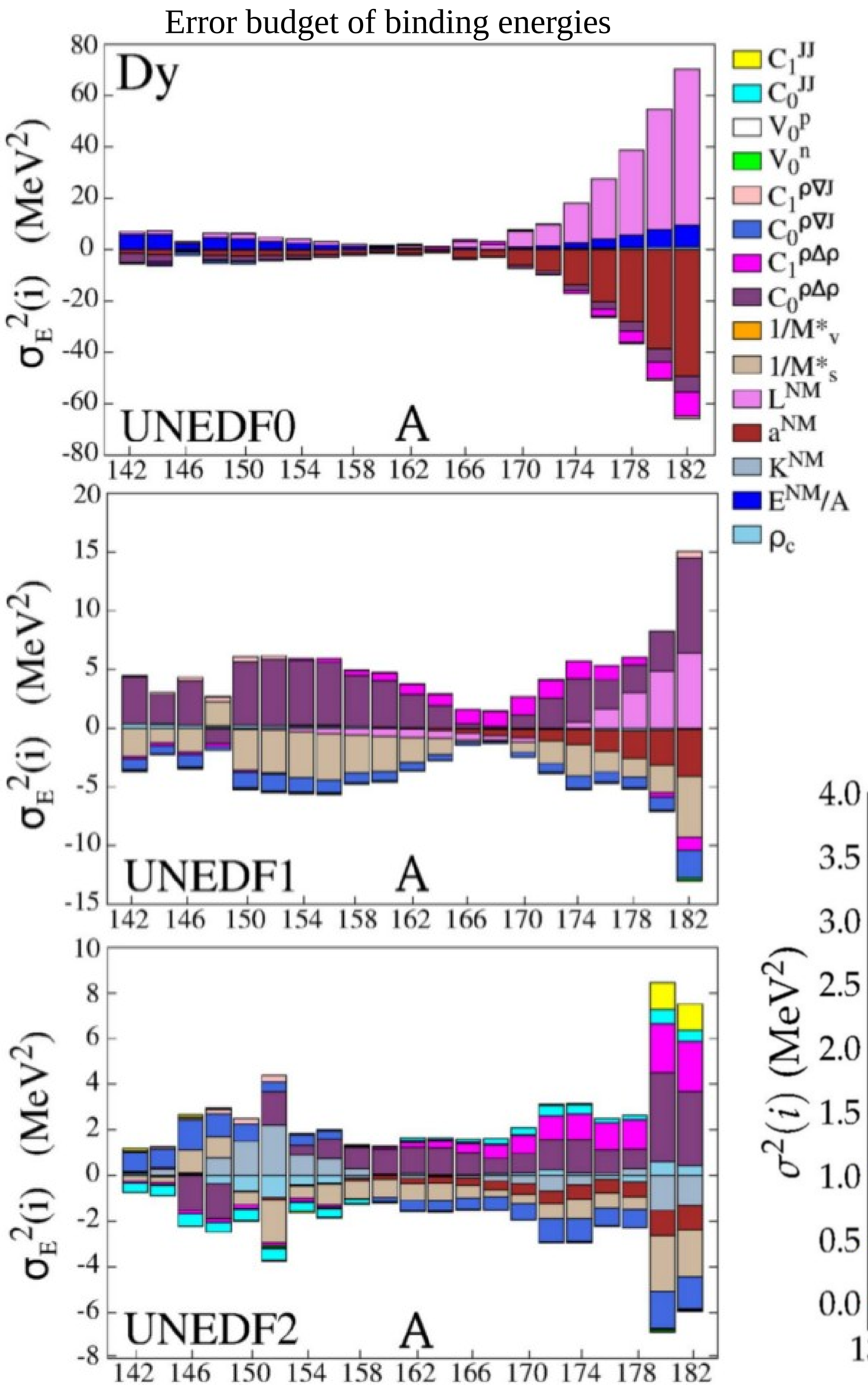


Uncertainty propagation in deformed rare earth nuclei, rms radius

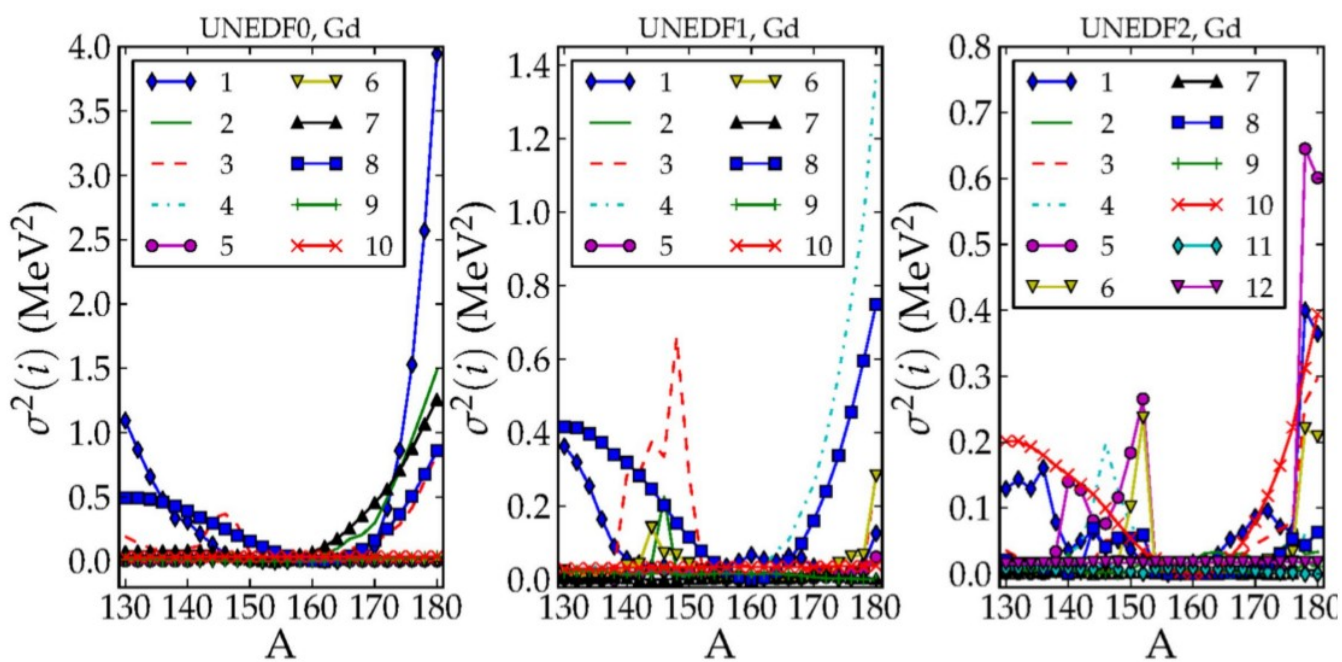
- Systematic error of radii and intrinsic quadrupole moment are strongly connected, as expected, since the presence of deformation increases radius
- Some of the nuclei close to semi-magicity are spherical, and thus the deformation uncertainty vanishes
- High values of uncertainty next to spherical nuclei are due to soft deformation energy landscape with respect of quadrupole deformation.



Uncertainty propagation in deformed rare earth nuclei, error budget



- By looking at the error budget, one can see which of the parameters contribute most on the statistical error
- With UNEDF0 only few parameters seems to be important ones, when looking at uncertainty of the binding energy.
- The eigenmode formalism also shows that only a few parameters contribute significantly. Most important eigenvectors mostly consists of those parameters which were found important in error budget
- With UNEDF1 and 2 more parameters become important



Finite range EDF

- UNEDF2 optimization indicated that novel approaches are needed
- Also, in future, access to spectroscopy and transition rates within DFT would be highly desired (i.e. beyond mean-field calculations)
- Almost all current EDFs are unsuited for beyond mean-field calculations (due to technical reasons, which are outside the scope of this workshop)
- Jyväskylä-Lyon-York approach: The finite range pseudopotential.
- Replaces zero-range Skyrme δ-term in EDF generator with a finite range term g_a with a length of *a* as

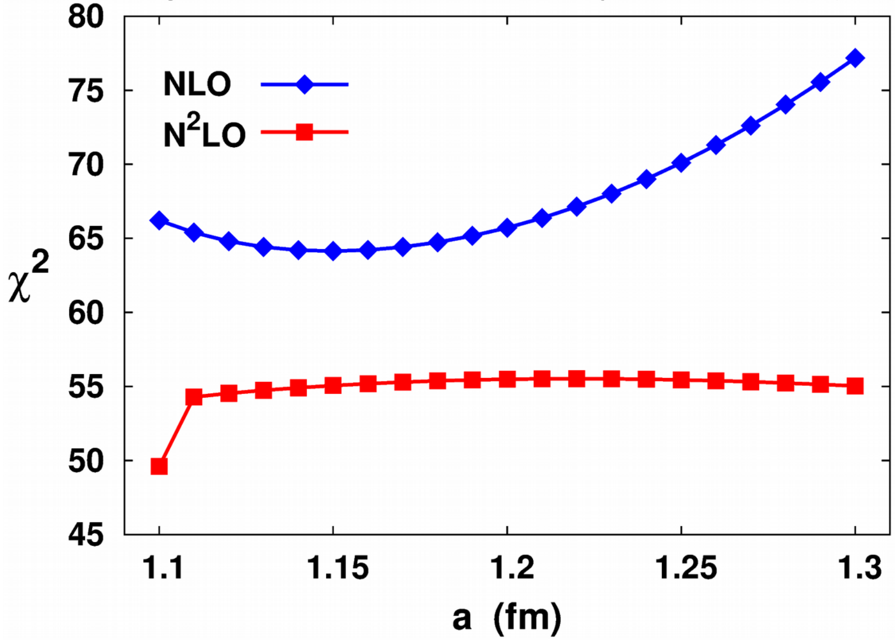
$$\delta(\boldsymbol{r}_i - \boldsymbol{r}_j) \rightarrow g_a(\boldsymbol{r}_i - \boldsymbol{r}_j)$$

  Includes also relative momentum operators up to order *2n*
- First introduced at F. Raimondi, et.al, J. Phys. G 41, 055112 (2014)
- First set of optimized parameters published recently: K. Bennaceur, A. Idini, J. Dobaczewski, P. Dobaczewski, M. Kortelainen, and F. Raimondi, J. Phys. G 44, 045106 (2017). Optimization at spherical HFB level
- Optimization data set contained masses of spherical nuclei, radii, pairing gaps, and some constraints on infinite nuclear matter. A zero range two-body term was introduced to obtain better pairing channel properties

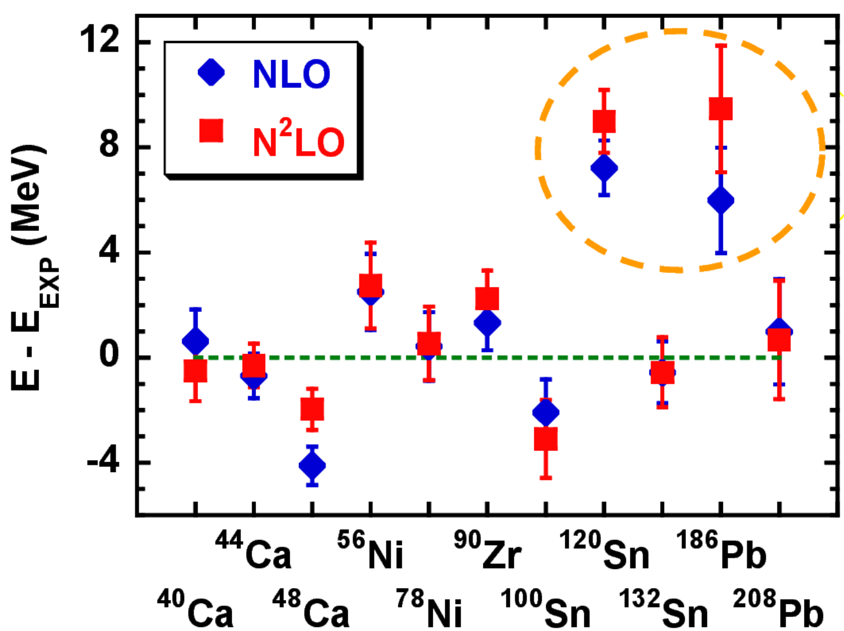
Results from first optimization

- At N2LO level, the χ^2 depends only weakly on the length scale *a*
- For spherical doubly-magic nuclei binding energy is usually rather well reproduced
- At mid-shell, small effective mass deteriorates predicted binding energies
- For deformed nuclei, propagated uncertainties become larger

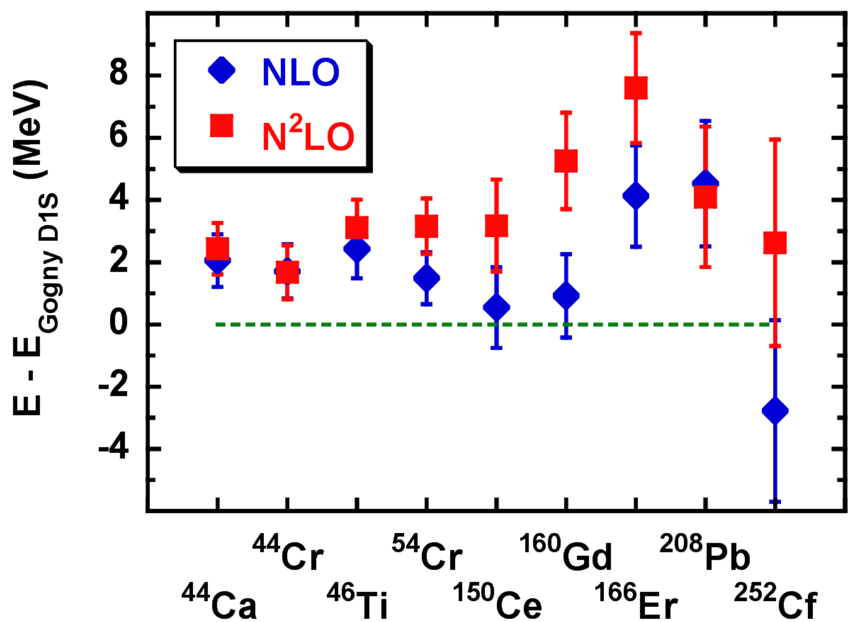
All figs. from K. Bennaceur, et.al, J. Phys. G 44, 045106 (2017)



Binding energies with propagated errors compared to experimental values



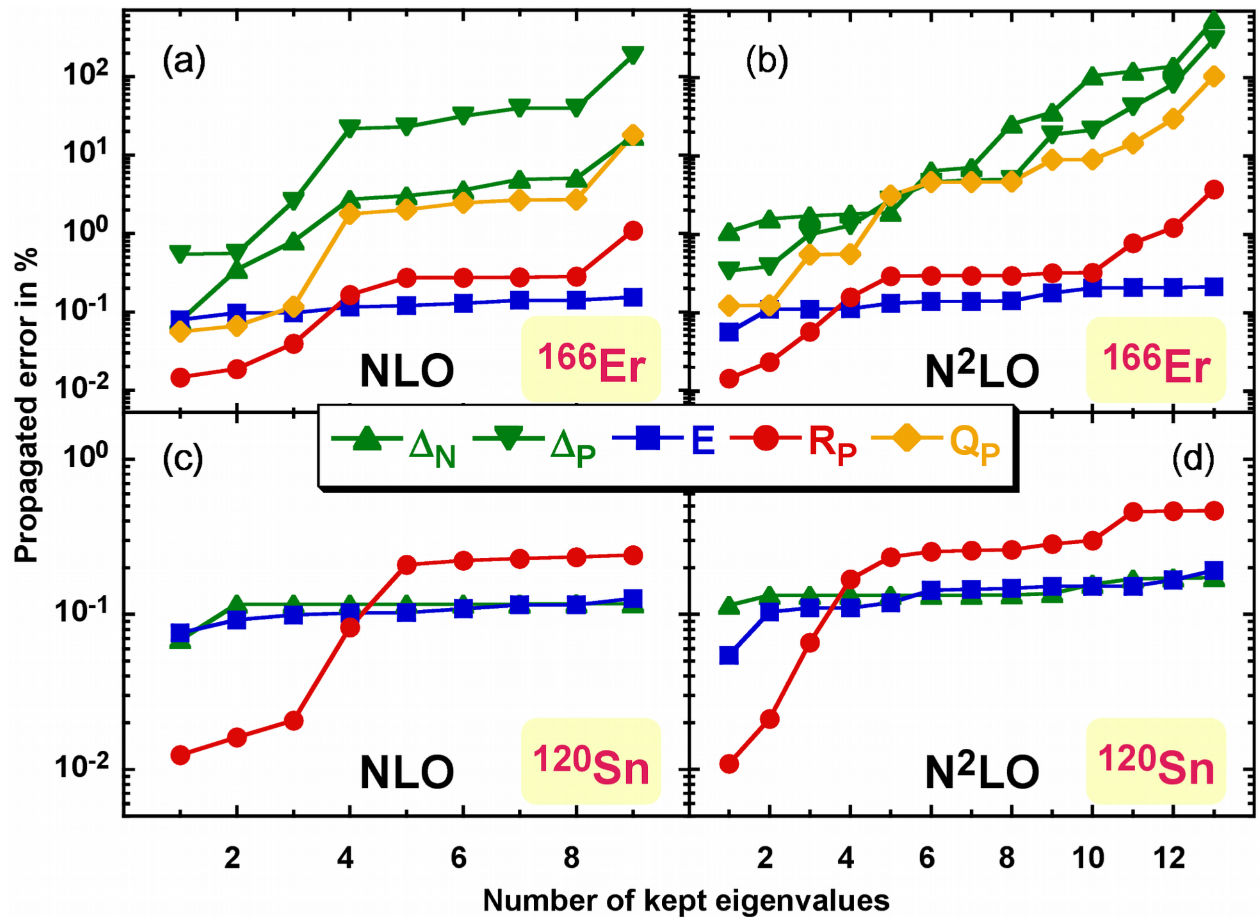
Binding energies with propagated errors compared to Gogny D1S



Propagated error in deformed nuclei

- A closer inspection shows that propagated error for some observables in deformed ^{166}Er become large
- Current input data can not constrain parameters which are strongly connected to these observables
- Future EDF parameter optimization done at deformed HFB level should fix some of these issues
- This can be done with newly developed HFB code called HFBtemp
- POUNDerS algorithm already coupled with HFBtemp (work done by Tiia Haverinen)

Propagated error as function of number of eigenvalues kept when computing covariance matrix. K. Bennaceur, et.al, J. Phys. G 44, 045106 (2017)



Conclusions and open questions

- Many UNEDF2 properties similarly good or slightly worse than with more specialized UNEDF0 or UNEDF1 when compared to exp. data.
- Sensitivity analysis shows that further major improvements for UNEDF2 are unlikely. The limits of Skyrme-like EDFs have been reached and novel approaches are required
- Finite range EDF shows promising results. This is an EDF suitable for beyond mean-field calculations
- Uncertainty quantification and other results tells that
  - Isovector parameters are more difficult to constrain, due to lack of good isovector data
  - Masses can constrain just some of the EDF model parameters
  - Fission isomers are good at constraining fission properties
  - The use of only spherical nuclei shows up as a relatively larger uncertainty with some the observables in deformed nuclei

Open questions:

- How can spectroscopic quality of a novel multi-reference (MR) EDF improved? What kind of data is required for such task?
  - Level scheme? (odd/even *N/Z*, rotational bands, vibrational states, open/closed shell)
  - EM transitions?
  - Beta transitions?
- Presently parameter adjustment is computationally practical only at the single-reference (SR) level. What kind of observables can be used at SR level to improve predictive power for spectroscopy at MR level?

Additional slides

Skyrme EDF

- The key ingredient of the nuclear DFT is the nuclear energy density functional (EDF)
- The EDF incorporates complex many-body correlations within the energy density constructed from the nucleon densities and currents
- Currently there are three major EDF variants in the market: Skyrme, Gogny and relativistic mean-field models. All of these contain a set of parameters which needs to be adjusted to empirical input
- Time-even and time-odd parts of the Skyrme EDF reads as

$$E_t^{even}(\boldsymbol{r}) = C_t^{\rho}\rho_t^2 + C_t^{\tau}\rho_t\tau_t + C_t^{\Delta\rho}\rho_t\Delta\rho_t + C_t^{\nabla J}\rho_t\nabla\cdot\boldsymbol{J}_t + C_t^{J}J_t^2$$

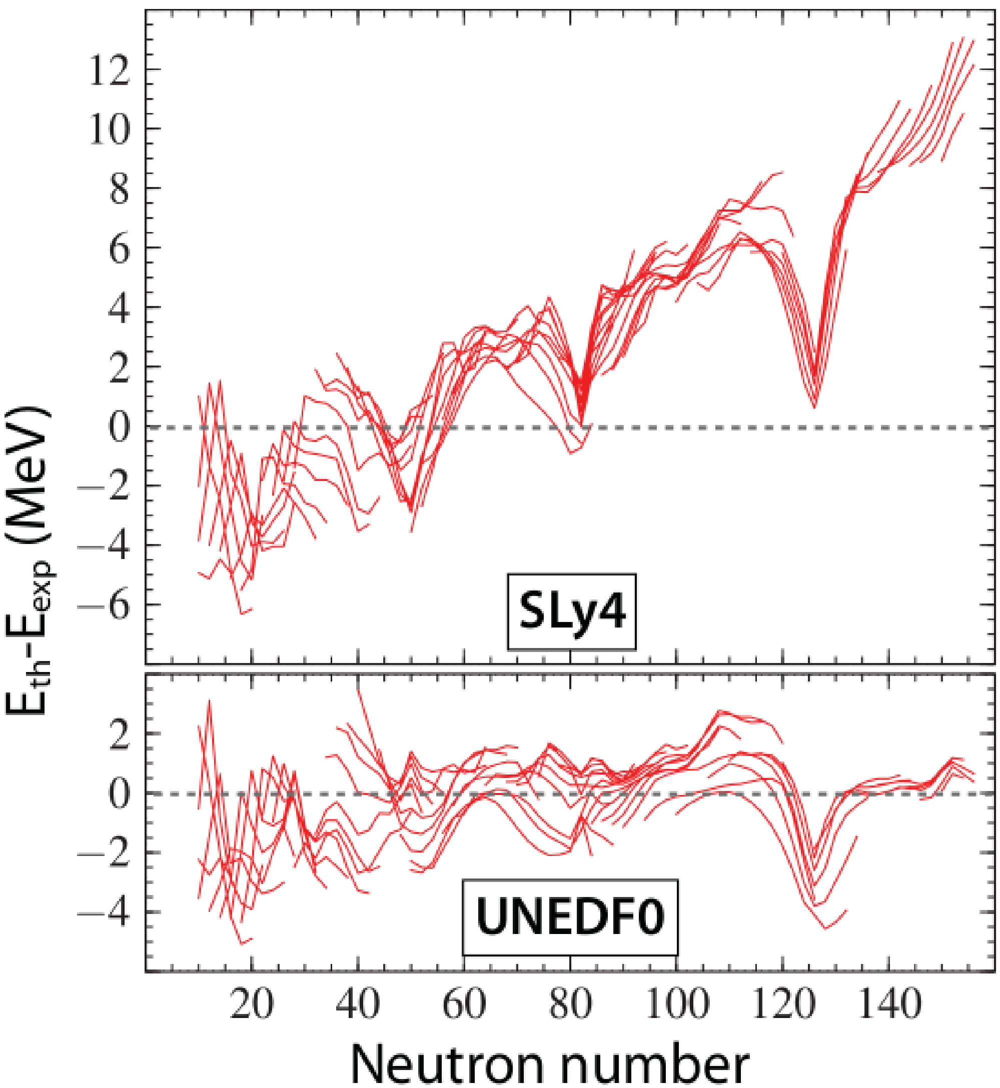
$$E_t^{odd}(\boldsymbol{r}) = C_t^{s}\boldsymbol{s}_t^2 + C_t^{j}\boldsymbol{j}_t^2 + C_t^{\Delta s}\boldsymbol{s}_t\cdot\Delta\boldsymbol{s}_t + C^{\nabla j}\boldsymbol{s}_t\cdot\nabla\times\boldsymbol{j}_t + C^{T}\boldsymbol{s}_t\cdot\boldsymbol{T}_t$$

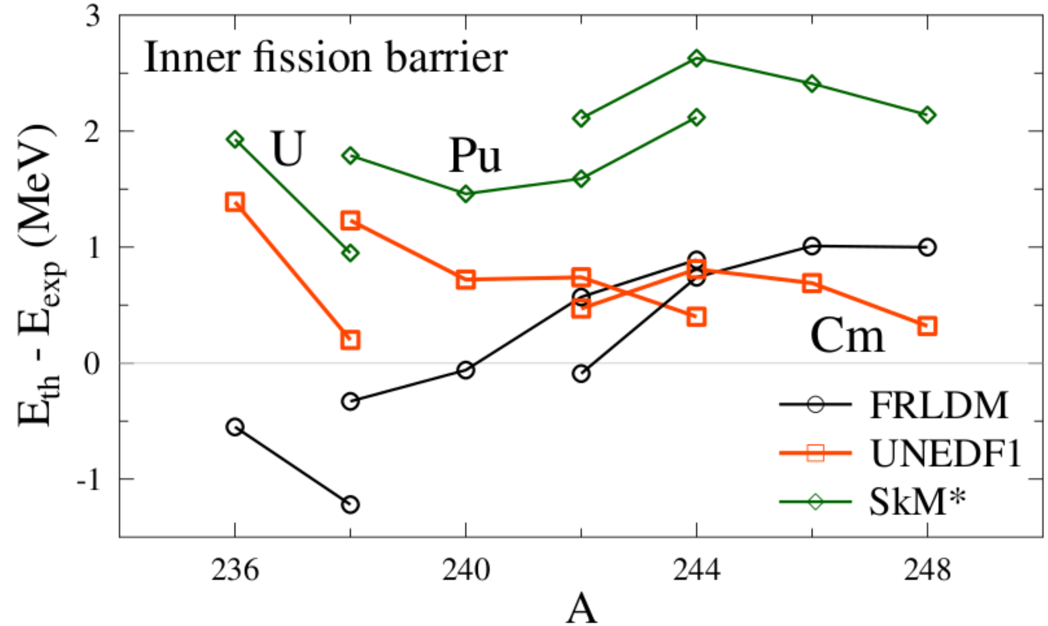
$$C_t^{\rho} = C_{t0}^{\rho} + C_{tD}^{\rho}\rho_0^{\gamma} \;,\quad C_t^{s} = C_{t0}^{s} + C_{tD}^{s}\rho_0^{\gamma} \;,\quad t=0,1$$

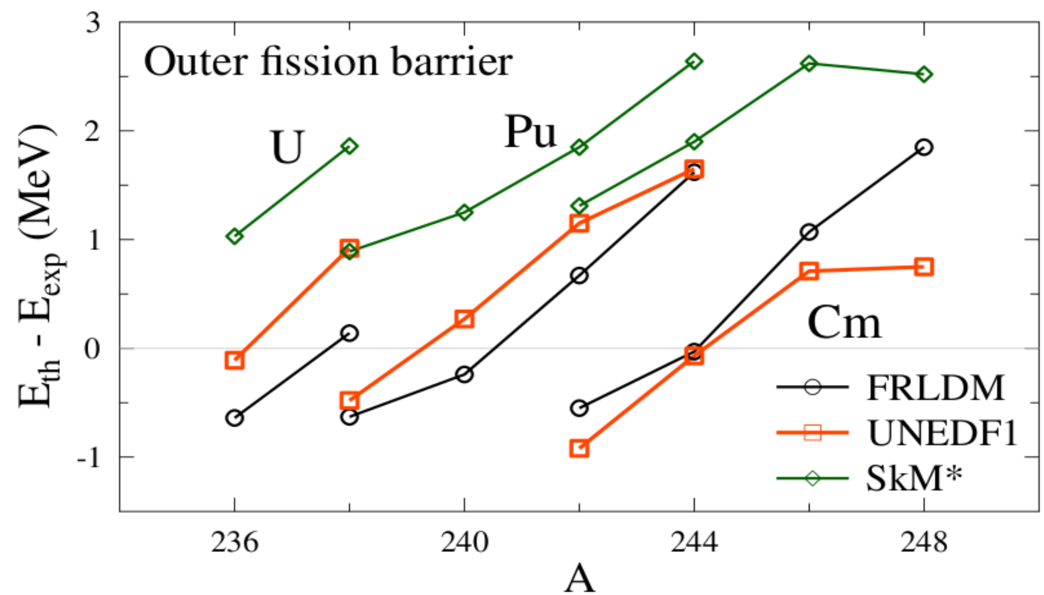
- Skyrme EDF is constructed from local densities ($\rho,\tau,\boldsymbol{J},\boldsymbol{s},\boldsymbol{j},\boldsymbol{T}$) (and their derivatives), and coupling constants multiplying each term
- For the HFB ground state of even-even nucleus, only time-even part contributes. For excited states, both parts are active

UNEDF0 and UNEDF1, performance

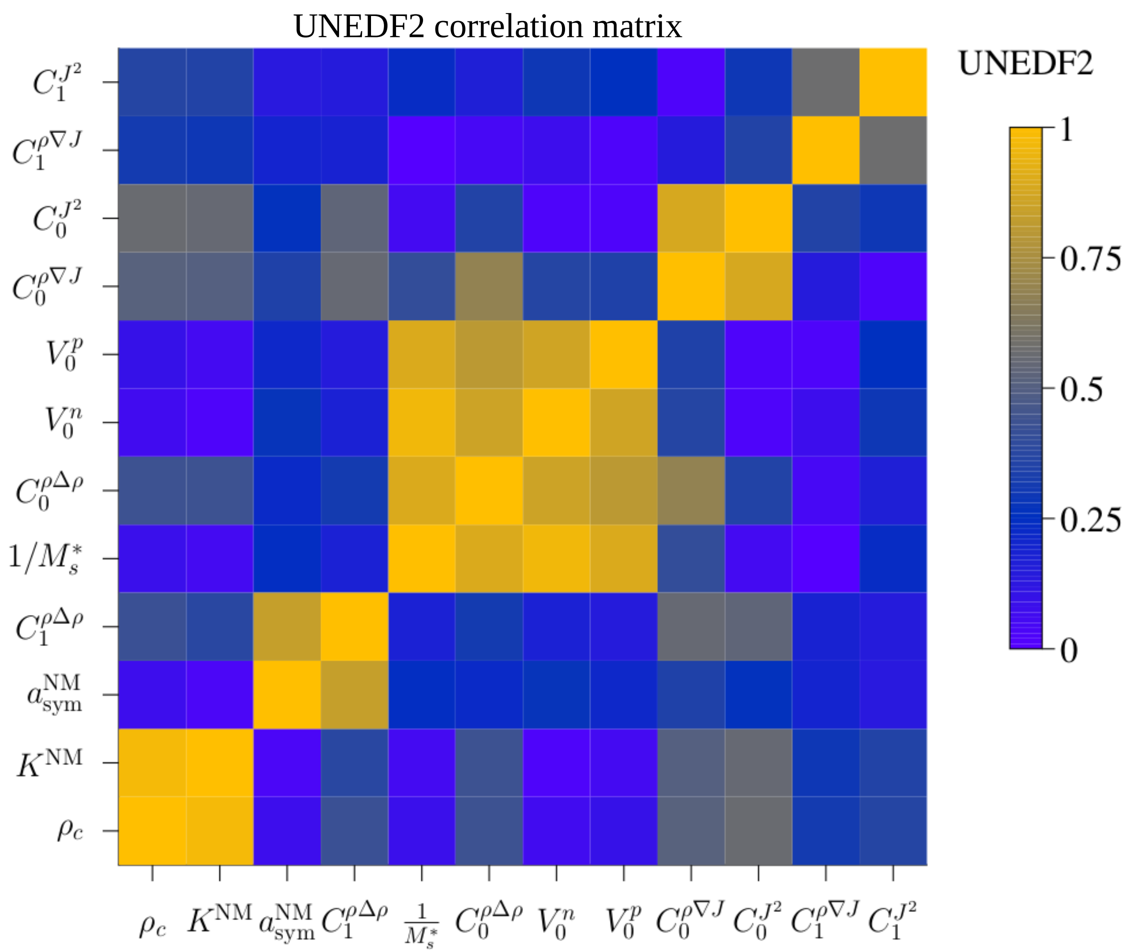
- UNEDF0 reproduces masses at level of rmsd 1.4 MeV (UNEDF1: 1.9 MeV)
- UNEDF1 reproduces actinide fission barriers better than SkM*

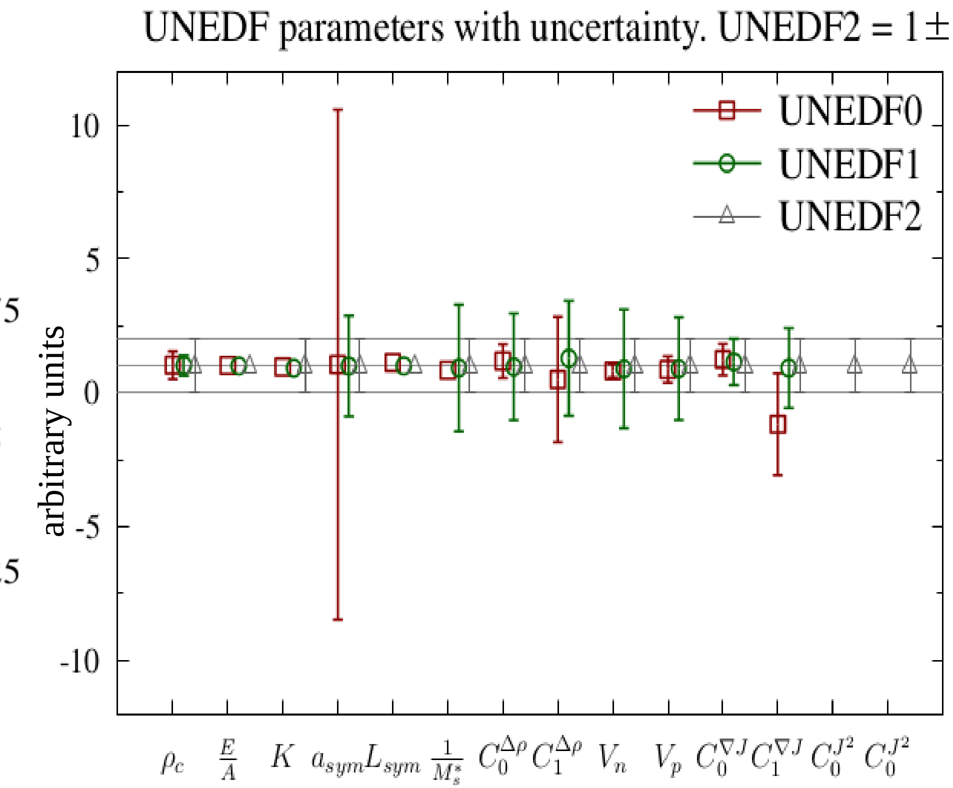


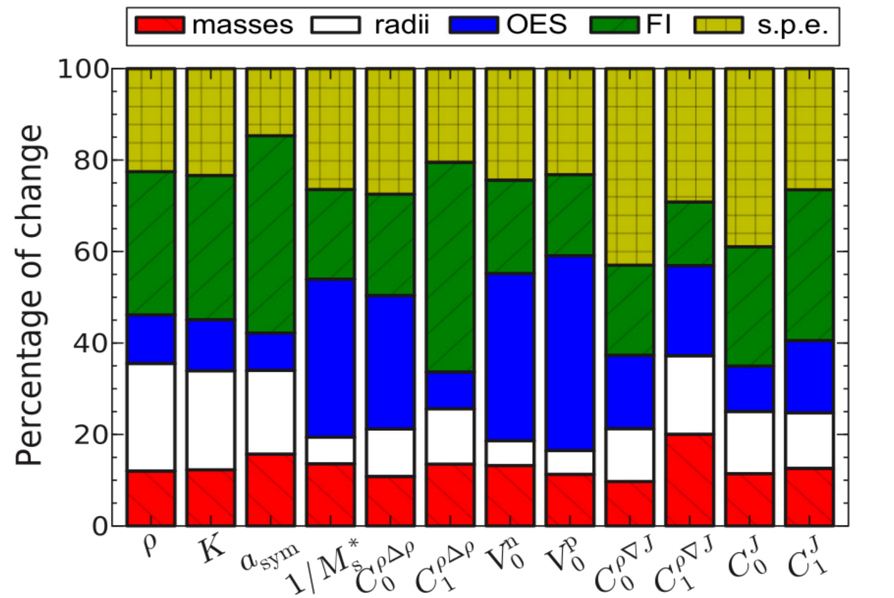




UNEDF sensitivity analysis







- UNEDF2 sensitivity analysis shows that UNEDF2 is better constrained that UNEDF0,1

Finite range EDF parameterization

Table 3. The NLO and N^2LO coupling constants of local pseudopotentials (3) and (7) regularized at $a = 1.15\,\mathrm{fm}$. (in $\mathrm{MeV\,fm}^{n+3}$) shown together with their statistical errors.

Order	Coupling Constant	NLO REG2c.161026	N^2LO REG4c.161026
$n=0$	$W_1^{(0)}$	41.678375 ± 0.6	3121.637124 ± 1.5
	$B_1^{(0)}$	-1405.790048 ± 4.3	-4884.029523 ± 1.8
	$H_1^{(0)}$	202.879894 ± 4.1	3688.310059 ± 2.9
	$M_1^{(0)}$	-2460.684507 ± 6.7	-5661.028710 ± 2.8
$n=2$	$W_1^{(2)}$	-79.747992 ± 4.2	547.802973 ± 1.9
	$B_1^{(2)}$	73.112729 ± 1.4	-319.513120 ± 1.3
	$H_1^{(2)}$	-681.295790 ± 3.2	-134.164127 ± 0.3
	$M_1^{(2)}$	-48.161707 ± 5.1	-318.407541 ± 0.6
$n=4$	$W_1^{(4)}$		2019.945667 ± 2.2
	$B_1^{(4)}$		-2365.956384 ± 1.6
	$H_1^{(4)}$		2310.445509 ± 1.8
	$M_1^{(4)}$		-2117.509518 ± 4.0
	W_{SO}	177.076480 ± 4.7	174.786236 ± 5.1

In addition a contact term

$$\mathcal{V}_\delta(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}_3, \mathbf{r}_4) = t_0 \left(1 + x_0 \hat{P}^\sigma\right) \delta(\mathbf{r}_{13})\delta(\mathbf{r}_{24})\delta(\mathbf{r}_{12})$$

with $x_0 = 1$, $t_0 = 1000$ MeV fm^3.

HFBtemp

- A modular HFB solver, in which one could freely combine various basis (axial, 3D Cartesian, ...) with various EDFs (Skyrme, finite range, ...), and later with other components (FAM-QRPA, PNP, AMP, …)
- Coding is done with c++ (2011 standard). Many external libraries used (Eigen, boost, yaml-cpp)
- Uses a lot of template programming structures
- Current implementation includes axial and 3D Cartesian harmonic oscillator bases, Skyrme EDF and finite range EDF for axial case
- Exchange part of the finite range potential is calculated from matrix product

$$h^{ex} = X^{\dagger}\left(V \circ \left(X \rho X^{\dagger}\right)\right) X$$

where ρ is the density matrix in configuration space, X is the matrix containing basis functions in the mesh, and V is the interaction

- OpenMP parallelization for a single HFB calculation, MPI parallelization available for multiple HFB calculations
- Good scaling with OpenMP

Speed-up: 16 shells, 32x32 mesh split to 8 sub-blocks, Intel and gcc compilers, Haswell cores